Folding transition of the triangular lattice in a discrete three–dimensional space

Emilio N.M. Cirillo
Dipartimento di Fisica dell'Università di Bari and
Istituto Nazionale di Fisica Nucleare, Sezione di Bari
via Amendola 173, 70126 Bari, Italy

Giuseppe Gonnella(*)
Theoretical Physics, Oxford University, 1 Keble Rd Oxford OX1 3NP, UK

Alessandro Pelizzola
Dipartimento di Fisica del Politecnico di Torino and
Istituto Nazionale per la Fisica della Materia,
c. Duca degli Abruzzi 24, 10129 Torino, Italy

Abstract

A vertex model introduced by M. Bowick, P. Di Francesco, O. Golinelli, and E. Guitter [Nucl. Phys. B **450**, 463 (1995)] describing the folding of the triangular lattice onto the face centered cubic lattice has been studied in the hexagon approximation of the cluster variation method. The model describes the behaviour of a polymerized membrane in a discrete three–dimensional space. We have introduced a curvature energy and a symmetry breaking field and studied the phase diagram of the resulting model. By varying the curvature energy parameter, a first-order transition has been found between a flat and a folded phase for any value of the symmetry breaking field.

PACS numbers: 05.50.+q (Ising problems); 64.60.-i (General studies of phase transitions); 82.65.Dp (Thermodynamics of surfaces and interfaces).

(*) Permanent Address:
Dipartimento di Fisica dell'Università di Bari and
Istituto Nazionale di Fisica Nucleare, Sezione di Bari, via Amendola 173, 70126 Bari, Italy

The macroscopic behaviour of membranes fluctuating in the euclidean space crucially depends on the microscopic characteristics of the system [1]. For example, a *fluid* membrane without self-avoiding interactions is always expected to be in a crumpled state [2], independently from the stiffness attributed to the membrane, while a rigid phantom [3] *polymerized* membrane, which is a network of molecules with fixed connectivity, is expected to be stable in a flat phase [4]. The existence of different classes of membrane systems suggests to consider specific lattice models paradigmatic for each class, which can be useful for analytical and numerical calculations. While many–component membrane systems can be sometimes expressed as Ising–like models [5], it is more difficult to describe the statistical behaviour of a single membrane in terms of usual lattice models with a local hamiltonian. In Ref. [6], a $D = 2$ vertex model has been introduced which describes the behaviour of a single phantom polymerized membrane with bonds of fixed length embedded in a discrete $d = 3$ space. The aim of this communication is to study the phase diagram of the membrane model of [6].

Models of polymerized membranes were introduced in [7], and studied using a Landau–Ginzburg evaluation of the energy of the system in [4, 8, 9, 10]. From the above studies, and from numerical simulations [11], it comes out that, when excluded volume effects are not considered, by varying the strength K of a bending energy term which favours flat configurations, a critical transition arises separating a flat phase at large K from a crumpled phase at small K.

Generally, the length of the bonds of a polymerized membrane can vary being subjected to elastic forces [4]. In [12] the simple case of a triangular network with bonds of fixed length embedded in a d–dimensional space has been first considered. This folding problem has been

studied in [13, 14, 15] in the case of a two–dimensional embedding space; here the normals to the triangles of the network can point only "up" or "down" in some direction. This model can be mapped on a 11–vertex model equivalent to a constrained Ising model with some spin configurations forbidden [13]; a first–order transition has been found to occur between a flat and a disordered phase [14, 15].

The more complicated problem of the folding of the triangular lattice in a three–dimensional embedding space has been formulated in [6], with the embedding space discretized as a face centered cubic lattice. In this model the plaquettes of the triangular lattice are mapped, by folding, onto those of a face centered cubic lattice, so that two adjacent plaquettes form an angle which can take up only four different values (see Fig. 1). In the following we introduce a term representing the stiffness of the network and study the phase diagram of the resulting model by applying the cluster variation method (CVM) in the same approximation used in [15].

The vertex model of [6] can be defined as follows. Two $\mathbf{Z}_2$ variables, named z_i and σ_i, are assigned to each plaquette of the triangular lattice, and hence to each site i of the dual hexagonal lattice. The relative values of these variables on adjacent plaquettes (say 1 and 2) determine the angle that is formed by the plaquettes, according to the following rules: for $z_1 = z_2$ and $\sigma_1 = \sigma_2$ we have no fold between the plaquettes; for $z_2 = -z_1$ and $\sigma_2 = \sigma_1$ we have an acute fold, with an angle θ such that $\cos\theta = 1/3$; for $z_2 = -z_1$ and $\sigma_2 = -\sigma_1$ we have an obtuse fold, with $\cos\theta = -1/3$; finally, for $z_2 = z_1$ and $\sigma_2 = -\sigma_1$ we have a complete fold, with the plaquettes lying one on top of the other (see Fig. 1).

It has been shown in [6] that the variables z_i and σ_i have to satisfy two constraints, or

folding rules, in order to describe a folding configuration over the face centered cubic lattice. Such folding rules take the form

$$\sum_{i=1}^{6} \sigma_i = 0 \bmod 3, \tag{1}$$

where the index i runs around a hexagon, and

$$\sum_{i=1}^{6} \frac{1 - z_i z_{i+1}}{2} \Delta_{i,c} = 0 \bmod 2 \quad c = 1, 2 \quad , \tag{2}$$

where $z_7 = z_1$ and

$$\Delta_{i,c} = \begin{cases} 1 & \text{if } \sum_{j=1}^{i} \sigma_j = c \bmod 3 \\ 0 & \text{otherwise} \end{cases} \quad i = 1, ..., 6, \; c = 1, 2 \quad . \tag{3}$$

We shall assume that a fold between two adjacent plaquettes has an energy cost, due to curvature, given by $-K \cos\theta$, where θ is the angle between the normal vectors to the plaquettes. In terms of our Ising–like variables such a term can be rewritten as $-K\sigma_i\sigma_j(1 + 2z_i z_j)/3$, manifestly symmetric under the global transformations $z_i \to -z_i, \forall i$ and $\sigma_i \to -\sigma_i, \forall i$. We will introduce also a term which breaks this symmetries, the analog of the magnetic field in the ordinary Ising model. In the two–dimensional case [14, 15] it was quite easy to define a symmetry–breaking field coupled to the direction of the normal to a plaquette, since there the spin variable associated to each plaquette denoted whether the normal was pointing up or down. In the present case and with the present parametrization this is no more possible, since the pair of values $\{z_i, \sigma_i\}$ does not determine the orientation of the plaquette. However, we are not interested in a true magnetic field, which cannot be given a physical meaning in this model, but just in a symmetry–breaking term, which can be realized in several ways. A simple choice, which favors only one of the four possible flat states (a flat state is easily seen to be characterized by the condition $\{z_i, \sigma_i\}$ independent of

i), leaving on the same ground the remaining three, is $-h\delta_{z_i,1}\delta_{\sigma_i,1}$. There are of course other possibilities, and in the following we shall consider one of these in order to show that the phase diagram is, roughly speaking, qualitatively independent of this choice.

We are thus led to consider the following hamiltonian (energies are given in units of $k_{\rm B}T$), defined on the dual hexagonal lattice:

$$\mathcal{H} = -\frac{K}{3}\sum_{\langle ij\rangle}\sigma_i\sigma_j(1+2z_iz_j) - h\sum_i \delta_{z_i,1}\delta_{\sigma_i,1}, \tag{4}$$

where the first sum is over nearest neighbor pairs.

As for the two–dimensional model, the phase diagram will be investigated by means of the hexagon approximation of the cluster variation method (CVM), which has been thoroughly described in [15]. This requires to introduce a hexagon density matrix $\rho_6(\{z_i,\sigma_i\})$, indexed by the hexagon configurations, a link density matrix ρ_2 and two site density matrices ρ_{1A} and ρ_{1B}, one for each of the two interpenetrating sublattices of the hexagonal lattice. Because of the folding rules Eqs. 1 and 2 one has not to consider $2^{12} = 4096$ hexagon configurations, but only 384, and hence 384 ρ_6 elements (this number may be slightly reduced by taking into account degeneracies, but this would lead to a more involved formulation). The link and site density matrices can be defined as partial traces of ρ_6 and, in analogy with [15], we can write the variational free energy density (in units of $k_{\rm B}T$)

$$\begin{aligned} f &= -\frac{K}{2}{\rm Tr}[(\sigma_1\sigma_2(1+2z_1z_2)\rho_2] - \frac{h}{2}[\rho_{1A}(z=1,\sigma=1)+\rho_{1B}(z=1,\sigma=1)] \\ &\quad +\frac{1}{2}{\rm Tr}(\rho_6\ln\rho_6) - \frac{3}{2}{\rm Tr}(\rho_2\ln\rho_2) + \frac{1}{2}\left[{\rm Tr}(\rho_{1A}\ln\rho_{1A}) + {\rm Tr}(\rho_{1B}\ln\rho_{1B})\right] \\ &\quad +\lambda({\rm Tr}\ \rho_6 - 1), \end{aligned} \tag{5}$$

where λ is a Lagrange multiplier which ensures the normalization of ρ_6 (and hence also of ρ_2

and ρ_{1A}, ρ_{1B}). This variational functional must, in general, be minimized numerically, and this can be done easily by an iterative method, as explained in [15].

At infinite temperature (or vanishing K and h) we obtain the entropy (per site) $S = \ln q$, where $q \simeq 1.42805$, in very good agreement with the transfer matrix estimate $q = 1.43(1)$ found in [6], although slightly lower than the best lower bound 1.43518 obtained from the analysis of two–dimensional folding in a staggered field [6]. Furthermore we obtain $\langle z_i \rangle_A = \langle z_i \rangle_B = 0$ and $\langle \sigma_i \rangle_A = -\langle \sigma_i \rangle_B \simeq 0.87456$, which, together with the values of the link density matrix elements, indicate a marked preference of the triangular lattice for obtuse and complete folds.

Let us now describe the main features of the phase diagram of the model Eq. 4, which has been obtained by means of the CVM and reported in Fig. 2, in the $K - h$ plane. The solid line separates the flat phase (high values of K and h, or low temperature) from the disordered, or folded, one (low values of K and h, or high temperature). The transition is of first order on the whole line; on the $h = 0$ axis the transition occurs at $K = 0.18548$, while on the $K = 0$ axis it occurs at $h = 0.49839$. The two phases can be distinguished by means of the energy–like correlation function $\langle \sigma_i \sigma_j (1 + 2 z_i z_j)/3 \rangle$, which is negative in the folded phase and saturates to 1 in the flat phase, indicating that the plaquettes are all parallel. As a consequence, in the flat phase the entropy vanishes and the free energy reduces to the internal energy contribution,

$$f_{\rm flat} = -\frac{3}{2} K - h. \tag{6}$$

The phase diagram of Fig. 2 is then easily obtained by comparing the value of the free energy of the disordered phase with $f_{\rm flat}$ above.

The first point to be discussed is that enlarging the embedding space has not turned the phase transition into a second order one, in contrast with what one could expect [6]. On the contrary, the first order character of the $h = 0$ transition seems to be enhanced in the three–dimensional case, as suggested by the jump in the energy–like correlation function, which is about 1.237 in the present case against 1.047 in the two–dimensional case. These features should be described correctly by the CVM approximation, as suggested by the good agreement with the transfer matrix results obtained both in the two–dimensional case [15] and, for the entropy at infinite temperature, in the present case.

The curvature term in Eq. 4, without the constraints Eqs. 1–2, corresponds to the anisotropic Ashkin–Teller model [16] with a particular choice of the parameters. We have studied in the CVM pair approximation the Ashkin–Teller model with the hamiltonian $\mathcal{H}_{\rm AT} = -K/3 \sum_{<ij>} \sigma_i \sigma_j (1 + 2 z_i z_j)$ and we have found two critical transitions at $K_{c1} = 0.824$ (where the symmetries $z \to -z$ and $\sigma \to -\sigma$ are separately broken, but their product is preserved) and $K_{c2} = 1.648$ (where even the product symmetry gets broken). In analogy with the result obtained in the two–dimensional case [15], we see that the introduction of defects which relax the constraints is necessary to smooth the transition.

Finally, it has already been observed before that the introduction of a symmetry–breaking field in the hamiltonian is not a trivial task as in the two–dimensional case [15]. It is therefore worth asking whether the basic features of our phase diagram depend on the choice of this field. For this reason we have considered a second model by introducing the h–field term in

the hamiltonian in the following way

$$\mathcal{H}_{\rm alt} = -\frac{K}{3}\sum_{\langle ij\rangle}\sigma_i\sigma_j(1+2z_iz_j) - \frac{h}{3}\sum_i\sigma_i(1+2z_i), \tag{7}$$

where h is non–negative. This amounts to let all the plaquettes interact, with an energy h, with a "ghost" plaquette which is fixed in the state characterized by $(z=1,\sigma=1)$. In Fig. 2 it is shown the phase diagram of the model Eq. 7 as well; the transition line is the broken one and is still a first order one. It is clear that the main features of the phase diagram have not been changed by replacing the old h–field term by the new one.

To summarize, we have studied in the CVM hexagon approximation the phase diagram of a vertex model which describes the folding of a triangular network onto a fcc lattice, subjected to a bending energy and a symmetry–breaking field. We have determined the folding entropy at infinite temperature, which is in very good agreement with a previous transfer matrix estimate, and the phase diagram of the model, which turns out to be qualitatively independent on the choice of the symmetry–breaking field. The flat and the folded phases are separated by a first–order transition, which is even stronger than that obtained with a two–dimensional embedding space. The lack of critical behaviour, which is expected for a polymerized phantom membrane, may be due to the particular choice of the discrete embedding space.

One of us (G.G.) thanks Amos Maritan for a discussion about the subject of this paper.

References

[1] See, e.g., *Statistical Mechanics of Membranes and Surfaces*, edited by D.R. Nelson, T. Piran, and S. Weinberg, (World Scientific, Singapore, 1989).

[2] L. Peliti and S. Leibler, Phys. Rev. Lett. **54**, 1690 (1985).

[3] Membranes where effects of excluded volume are not considered are sometimes called phantom membranes.

[4] D.R. Nelson and L. Peliti, J. Phys. (France) **48**, 1085 (1987).

[5] See, e.g., A. Cappi, P. Colangelo, G. Gonnella and A. Maritan, Nucl. Phys. B **370**, 659 (1992).

[6] M. Bowick, P. Di Francesco, O. Golinelli and E. Guitter, Nucl. Phys. B **450**, 463 (1995).

[7] Y. Kantor and D.R. Nelson, Phys. Rev. Lett. **58**, 2774 (1987); Phys. Rev. A **36**, 4020 (1987).

[8] M. Paczuski, M. Kardar, and D.R. Nelson, Phys. Rev. Lett. **60**, 2638 (1988).

[9] F. David and E. Guitter, Europhys. Lett. **5**, 709 (1988).

[10] J.A. Aronovitz and T.C. Lubensky, Phys. Rev. Lett. **60**, 2634 (1988); M. Paczuski and M. Kardar, Phys. Rev. A **39**, 6086 (1989).

[11] M. Baig, D. Espriu and J. Wheater, Nucl. Phys. B **314**, 587 (1989); R. Renken and J. Kogut, Nucl. Phys. B **342**, 753 (1990); R. Harnish and J. Wheater, Nucl. Phys. B **350**, 861 (1991); J. Wheater and P. Stephenson, Phys. Lett. B **302**, 447 (1993).

[12] Y. Kantor and M.V. Jarić, Europhys. Lett. **11**, 157 (1990).

[13] P. Di Francesco and E. Guitter, Europhys. Lett. **26**, 455 (1994).

[14] P. Di Francesco and E. Guitter, Phys. Rev. E **50**, 4418 (1994).

[15] E.N.M. Cirillo, G. Gonnella and A. Pelizzola, Phys. Rev. E, in press.

[16] See, e.g., R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London 1982).

Figure Captions

Figure 1: The four possible foldings of two adjacent plaquettes of the triangular lattice embedded in a fcc lattice are shown. From the left to the right and from the top to the bottom: no fold, acute fold ($70^0 32'$), obtuse fold ($109^0 28'$) and complete fold. The dots represent the vertices in an elementary cell of the fcc lattice.

Figure 2: Phase diagram in the $K - h$ plane: the solid and dashed lines correspond to hamiltonians $\mathcal{H}$ and $\mathcal{H}_{\rm alt}$, respectively.